AB INITIO TREATMENT OF MAGNETIC ANISOTROPY IN MONO- and BI-NUCLEAR COMPLEXES

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Since the early 1990s, single-molecule magnets SMMs have generated continuous interest of a large scientific community as their properties proved to be challenging from both technological and fundamental points of view. Their main remarkable property is the slow relaxation of their magnetization at low temperature, which is interpreted in terms of a lift of degeneracy of the *Ms* components of the ground state and to a long lifetime of the Ms_{max} components. The microscopic origin of magnetic anisotropy is due to synergistic effects between spatial anisotropy and relativistic effects, in particular spin-orbit coupling. This presentation recalls some qualitative challenges of the field. Then it presents the rational steps of a new method of extraction of magnetic anisotropy parameters which has successfully been applied to mono- and bi-metallic compounds [1,2,3,4,5]. The method is also used to question the validity of anisotropic spin Hamiltonians which are commonly used both to interpret the measured spin properties of anisotropic compounds (EPR spectroscopy) and to model these properties.

References

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